# WATER

## Energy and Environment Compendium

Los Alamos
NATIONAL LABORATORY

# WATER

## Energy and Environment Compendium

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LALP-04-026

April 2004

Los Alamos
NATIONAL LABORATORY

Los Alamos NM 87545

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# Water Research at Los Alamos National Laboratory

Water resource management has become a critical issue worldwide, the result of dwindling potable water supplies and expanding populations into regions with limited water reserves. In the United States, it is critical for national security and a strong economy that we ensure safe, dependable water supplies can meet the country's changing population demographics. Through its research in atmospheric, surface, and subsurface water, Los Alamos National Laboratory (LANL) has conducted focused efforts to resolve risks and problems associated with water resources. The Laboratory has also guided technology developments to ensure dependable water resources and to protect human health and the environment.

With a cohesive strategy, the LANL team pursues water research on multiple scales, from atoms to oceans, and across a broad range of issues, from ensuring clean, adequate water supplies to assessing water security risks and understanding the effects of societal shifts on water demands.

## Current Scientific Challenges in Water Research

Creating integrated models based on acquired data is necessary to gain insight into water resource issues and to assist with trend prediction. Predictive decision analysis techniques can help decision makers analyze uncertainties, predict scenarios, understand trade-offs, and implement optimized solutions. Applying research results to real-world situations to protect and conserve our water resources, and educating both policymakers and the general public about water issues are the final goals of Los Alamos's water research programs.

## Problem-Solving Capabilities in Water Research

- **Modeling and Simulation**—Los Alamos has expertise in modeling water on all scales, from models of atomic and molecular interactions to coupled models of river basins to integrated models of ocean currents and ice flow patterns.
- **High-Performance Computing**—Los Alamos researchers have high-performance computing facilities to execute complex simulations.
- **Observational and Experimental Methods**—The Laboratory has extraordinarily sophisticated observational and experimental methods, and has gathered data on atmospheric water, sediment, surface water, and groundwater.
- **Analytical Chemistry**—Los Alamos has the analytical chemistry expertise to solve key water quality issues.
- **Multidisciplinary Approaches to Complex Systems**—Exceptionally diverse multidisciplinary teams solve scientific and engineering challenges.
- **Data Management and Analysis**—Legacy databases are valuable resources to water quantity, quality, and interaction research.
- **Pollution Prevention**—Scientists and engineers at Los Alamos National Laboratory have long been involved in green chemistry activities and experiments involving various chemical and radioactive species, allowing them to develop expertise in minimizing the impact of these species on the environment.
- **Decision Analysis**—Procedures developed by the Laboratory to support military and national security decisions can be applied to help researchers and policymakers make more informed decisions regarding water issues.
- **Security and Threat Analysis**—The Los Alamos team has decades of experience in national and international nuclear security that can be applied to protect the civilian water supply.

# DOE Water Cycle Pilot Study

## The Challenge: Understanding Regional and Global Hydrological Cycles

Los Alamos National Laboratory co-chaired the committee that produced the Department of Energy's (DOE) Water Cycle Initiative Research Strategy, which defined the agency's role in the U.S. Global Change Research Program's Water Cycle Study. The successful collaboration between Los Alamos and the larger team led to a pilot study funded by the DOE. The Water Cycle Pilot Study is focused on the Whitewater River basin in Kansas, which is part of the DOE ARM (Atmospheric Radiation Measurement) Southern Great Plains site. It began with the goal of improving model parameters and our physical understanding of the water cycle through process studies, new observational methods, and field sites that provide continuous long-term data streams.

Another goal is to couple models in a high-performance computing environment, link domain models across processes (physical, chemical, geological, and biological) and scales (global, regional, local) and to provide a modeling and testing environment for DOE and the U.S. Global Change Research Program's research efforts.

Above: View of the landscape in the Whitewater River Basin, Kansas.

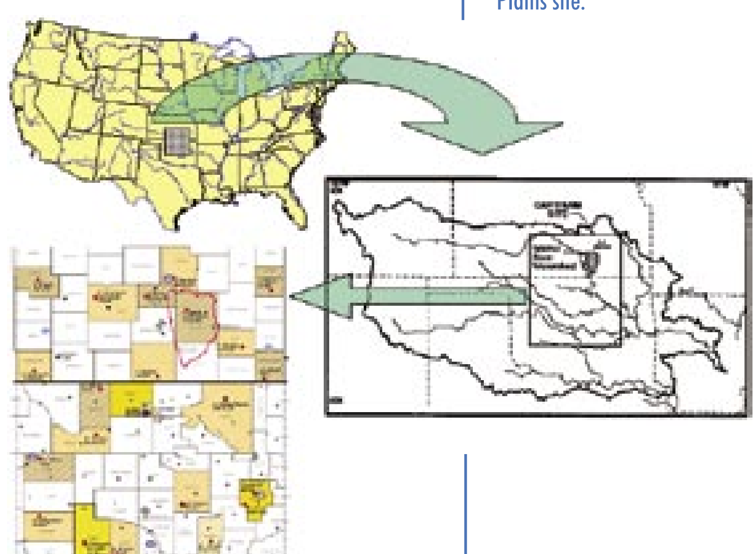
## Los Alamos Innovation: Coupling Complex Models

The Pilot Study was built upon the complementary abilities of the larger team. Los Alamos National Laboratory contributed its high-performance computing and existing capabilities in coupling regional atmospheric and hydrologic models.

Below: A map of the Whitewater River Basin within the DOE/ARM Southern Great Plains site.

## The Impact: Predicting the Future of Water Resources

Over the course of the Pilot Study, researchers are collecting and analyzing data to assess and predict the effects of climate variability and land use change on water resources. When the pilot study is completed, it will have created coupled models in a high-performance computing environment and demonstrated the capability of integrated teams to address complex problems.



# Evapotranspiration Mapping and Riparian Consumptive Use

## The Challenge: Addressing a Critical Unknown Variable of Riparian Vegetation Water Use

The Bureau of Reclamation (BOR) has identified riparian vegetation consumptive use of water, known as "evapotranspiration," as a critical unknown variable in understanding surface and subsurface water resources on watersheds such as the Rio Grande. Previous studies used point sensors to make evapotranspiration measurements, but uncertainty in the spatial variability precluded definitive results. To overcome this problem, the BOR in Albuquerque funded a water flux mapping study and requested Los Alamos participation. The ongoing research measures the water use of salt cedar and cottonwood, tree species common to riparian zones in the southwest, to determine if they differ in their water use. The goal is to improve water management on the Rio Grande.

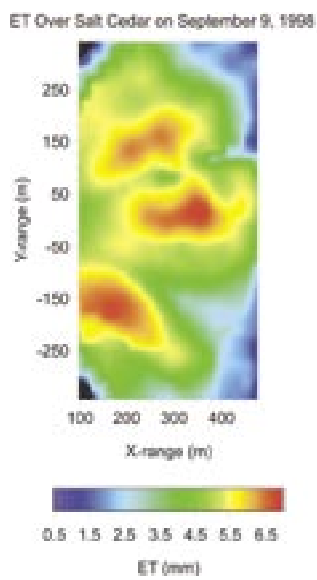
## Los Alamos Innovation: Using LIDAR to Measure Evapotranspiration

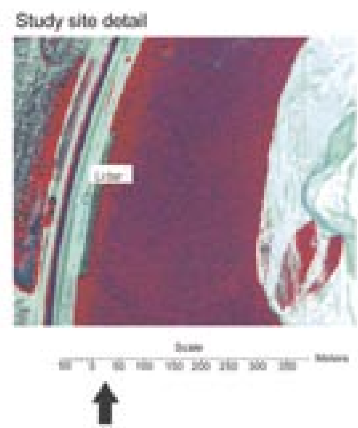
In coordination with universities in New Mexico and nationwide, the Laboratory has assembled an interdisciplinary measurement and analysis team to field, operate, and analyze data with its unique mobile scanning Raman water vapor LIDAR (Light Detection and Ranging) technology. LIDAR can measure evaporation thoroughly and accurately across time and space.

## The Impact: Better Management of River Basins

The collaboration will help to better understand evapotranspiration at selected riparian sites along the Rio Grande and will result in the development of spatial maps of evapotranspiration over the Bosque del Apache study site to represent selected phonological periods in the riparian vegetation growth patterns. In addition, quantifying the spatial and temporal variability in evapotranspiration on local micro-scales will be possible as will the translation of spatial and temporal variability terms to an evapotranspiration model for sub-sections of the Rio Grande. The accurate measurement and modeling of this key variable will improve the management of river basins.

Using the scanning capability of the mobile Raman water vapor lidar, LANL has developed a water vapor flux mapping system. The first image shows the spatial variability of evapotranspiration for a typical day in September over the salt cedars on the banks of the Rio Grande River; for reference, a false color infrared air photo of the site is shown at right.



# Semi-Arid Hydrology and Riparian Areas

## The Challenge: Integrating Teams to Tackle Complex Hydrology Issues

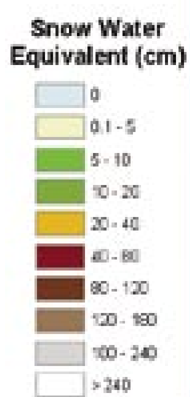
In 2001, the National Science Foundation (NSF) Science and Technology Center for Sustainability of Semi-Arid Hydrology and Riparian Areas (SAHRA) began operations with a mission to promote sustainable management of water resources in semi-arid regions. Led by the University of Arizona, other participants include the University of New Mexico, New Mexico Tech, University of California Riverside, University of California Los Angeles, other universities, and government agencies. Los Alamos National Laboratory is a partner in the SAHRA multidisciplinary team, and leads the effort in multi-resolution integrated modeling of basin-scale processes.

## Los Alamos Innovation: Integrating High-Resolution Models

Los Alamos's unique capabilities in high-performance computing and modeling have resulted in the creation of an integrated, high-resolution model to understand and predict the effects of climate variability and land use change on the water balance. LANL's participation in SAHRA has allowed for rapidly integrated computer codes that simulate atmosphere, surface, and groundwater components. The Parallel Applications Workspace—developed at Los Alamos—has also been used to couple the Regional Atmospheric Modeling System and the Los Alamos Distributed Hydrologic System with minimal changes to the two application codes. This model simulates the Rio Grande Basin, where it is now being tested.

One major interface that has not been exploited in the past is the socio-economic modules. This interface is challenging, but necessary for models to be successful in supporting decisions. Without it, policymakers can fail to see the strong personal and politically sensitive reasons behind studying and protecting the hydrology of semi-arid riparian areas.

Simulated distribution of snow water equivalent across the Rio Grande Basin above Cochiti Reservoir.


## The Impact: Better Management of Water Resources in Semi-Arid Regions

Los Alamos's participation in SAHRA has provided the Laboratory with an opportunity to apply its expertise to critical water resource problems in New Mexico and the southwestern United States.



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# Española Basin Aquifer Model

## The Challenge: Sustaining Groundwater Quantity and Quality

Maintaining a dependable and high-quality water supply in arid and semi-arid regions is a growing national concern, particularly because of prolonged drought conditions. In New Mexico, where groundwater provides more than 80 percent of public water supplies, Los Alamos National Laboratory and the surrounding area (Los Alamos, Española, Santa Fe, and many pueblos) rely on the Española Basin Aquifer. Declining water levels in the basin are of great importance to the Laboratory because of the implications for a sustainable water supply and because of the potential decline in groundwater quality.

## Los Alamos Innovation: Large-Scale Yet Detailed 3-D Models

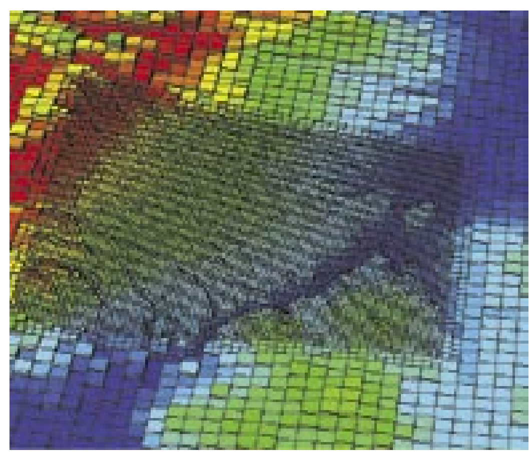
With an on-site technical team of geologists, geophysicists, geochemists, and hydrologists, Los Alamos is developing a unique, multidisciplinary approach to address basin-scale hydrologic questions, such as:

- How much high-quality water is in storage in the regional aquifer and how rapidly is this reservoir being depleted?
- What impact do aquifer withdrawals have on surface water flow?
- How will the drought affect groundwater supplies?

Addressing these questions requires developing a simulation model that is sufficiently large in scale to encompasses the entire aquifer (approximately 100 square kilometers) but also sufficiently detailed as to capture small-scale variations in hydrostratigraphy and stresses on the aquifer because of pumping. The high-performance computing facilities and flow and transport codes at Los Alamos provide a cornerstone for developing models with high resolution and tight coupling between hydrologic and geochemical processes. Using these tools, a large body of geologic, geophysical, and geochemical data has been integrated into a sophisticated 3-D model of the basin aquifer. Los Alamos has also developed and applied statistical methodologies for applying model predictions in decision-making contexts. The modeling and analysis tools can:

- Predict the rate of future water level declines due to pumping;
- Predict the ultimate fate of contaminants in the regional aquifer;
- Optimize data collection in deep boreholes being drilled at the Los Alamos site;
- Evaluate the adequacy of groundwater monitoring strategies;
- Estimate the uncertainty of model predictions; and
- Visualize flow paths and aquifer characteristics in 3-D.

Close up image of White Rock Canyon within the Española Basin numerical grid.



## The Impact: Better Resource Management Locally and Beyond

Detailed analysis of these problems is important not only for the study area, but also regionally and globally. Benefits of the modeling include assisting Los Alamos National Laboratory and surrounding communities in evaluating potential threats to water quality and rates of aquifer depletion. The modeling and prediction methods developed for the Española Basin can be transferred to other regions to assist in widespread national and global resource management.



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# Jemez y Sangre Water Planning Council

## The Challenge: Chairing the Council to Implement the Regional Water Plan

In 1987 the New Mexico legislature enacted a statute enabling regions in the state to plan their water future, and in 1998 the Jemez y Sangre Water Planning area was established. Water planning was initiated at the regional level so that unique characteristics of each region would be equally protected. As a major water user in the planning region, Los Alamos National Laboratory actively participated in developing the Jemez y Sangre Regional Water Plan. The Interstate Stream Commission accepted the plan in April 2003. The Council is in the initial phase of implementing the plan.

## Los Alamos Innovation: Providing Leadership in Water Resource Issues

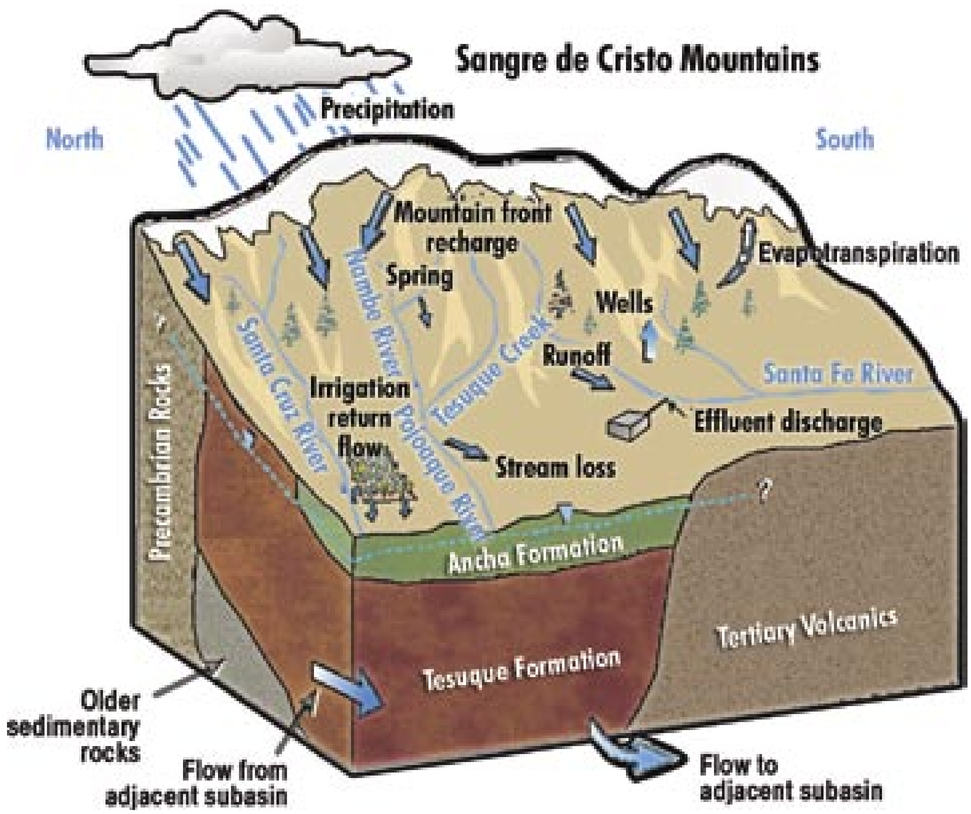
The Laboratory chairs the Water Planning Council, and also participates in the subcommittees that focus on understanding sustainable ground and surface water use, provide education, and assess implementation performance.

The Laboratory also chairs the executive committee. Los Alamos's participation in the Jemez y Sangre Council provides additional insight into New Mexico's water resources issues and also provides opportunities to use Laboratory capabilities to understand and address water resource issues of the state and region.

## The Impact: Securing Water Supplies for the Next 60 Years

The regional water planning efforts of the Jemez y Sangre Council resulted in the development of an inventory of the quantity and quality of water resources in the Jemez y Sangre region. Projected water resource demands, responding to a range of conditions, were calculated as a result of these efforts.

The council also recommended alternatives to close the projected gap between supply and demand through 2060 by managing and conserving the region's available water supplies under existing rights, water supplies, interstate agreements, and court decrees. The sum of these efforts will help secure a sustainable water supply for future generations by implementing recommendations in the water plan.




Conceptual model of Jemez y Sangre water planning region.

# New Mexico Governor's Blue Ribbon Water Task Force

## The Challenge: Investigating the Current Water Policies and Laws of New Mexico

New Mexico is an arid state with a limited amount of water available for use by its citizens. To ensure an adequate water supply for generations of New Mexicans to come, long-range planning relating the State water use and policies is necessary. To meet New Mexico's planning needs, the Blue Ribbon Water Task Force was established.

## Los Alamos Innovation: Science-Based Advice for State Water Planning

As requested by Governor Bill Richardson, Los Alamos National Laboratory provides two members to this Task Force. The purpose of the Task Force is to investigate and engage in discussions regarding current water policies and laws implemented within New Mexico.

The council has also been tasked with advising the State Engineer, Interstate Stream Commission, and any other relevant state agencies, regarding water policy and laws in relation to the population and implementation of the State Water Plan. It also provides the Governor with its recommendations every November and provides copies to the State Engineer and Interstate Stream Engineer.

The Blue Ribbon Water Task Force will provide water policy and law recommendations annually to New Mexico's Governor.

## The Impact: Science, Law, and Public Policy Working in Concert

Water management goes beyond understanding physical, natural systems alone. The Blue Ribbon Task Force will help untangle the web of legal, economic, and policy issues that are intertwined with scientific and technological solutions.

# ZeroNet Water

## The Challenge: Increasing New Mexico's Power Without Increasing Water Usage

New Mexico has serious water problems that will be exacerbated by continued population growth and a potential long-term drought. The ZeroNet Water-Energy Initiative's goal is, by 2010, to meet New Mexico's increasing electric power demand without increasing water use for power plant cooling.

## Los Alamos Innovation: Creating Multiple Options Through Multiple Partners

Los Alamos National Laboratory, The Electric Power Research Institute, and the Public Service Company of New Mexico (PNM) together have created ZeroNet. ZeroNet provides support tools to manage competition for water resources while accelerating current technological innovations. To further these initiatives, ZeroNet has pursued an aggressive technology transfer and implementation schedule.

Partners from industry, other national laboratories, universities, and state and federal governments ensure capabilities are leveraged to provide multiple water use solutions. ZeroNet takes a comprehensive and integrated approach by incorporating the following program elements:

- Degraded water use—alternative water sources for cooling systems;
- Integrated modeling and management scenario assessment—approaches include Watershed Analysis Risk Management Framework and Integrated Basin Model;
- Economic, market, and risk analysis;
- Water efficiency, conservation, recycling, and renewables;
- Monitoring and measurement;
- Advanced cooling; and
- Land management–piñon, juniper and upland forest thinning, removal of non-native riparian species.

PNM's San Juan Generating Station near Farmington, N.M. will serve as a test site for the ZeroNet Initiative.

## The Impact: Adequate Supplies of Electricity and Water for the Future

This initiative will deliver new electric power capacity in New Mexico with "zero net" freshwater withdrawals while ensuring a stable water resource for energy producers. Energy costs will be reduced because clean, affordable water can be provided. Los Alamos will also create a detailed source of water and energy information to aid the public and policy-makers and will provide targeted technological solutions and technology transfer opportunities. The quality of the nation's fresh water supply will be improved and competition between energy producers and other water users will be alleviated. The result will be an innovative model that can be adapted for other states and regions.

# Los Alamos Hydrogeologic Workplan

## The Challenge: Characterizing Los Alamos's Hydrogeological Setting

In response to a request from the New Mexico Environment Department, the Laboratory developed a hydrogeologic workplan that details activities to be performed over a 7-year schedule for a site-wide hydrogeologic characterization. Implementing the workplan would provide sufficient information to adequately design and install additions to the groundwater-monitoring network for the site. Los Alamos based the hydrogeologic workplan on the application of the Environmental Protection Agency Data Quality Objective (DQO) process to optimize the data collection design. The workplan depends on an iterative approach—collecting data from a specific borehole and well that will be analyzed and interpreted for sound decision-making on future data collection activities, thereby allowing for project economies and selection of appropriate DQOs.

## Los Alamos Innovation: Producing Sophisticated Models to Understand Site Hydrogeology

The Laboratory develops discrete sampling and analysis plans for each well; these plans detail the DQOs and well design. The completed wells are typically constructed with multiple screens, where instrumentation is used to allow discrete sampling and pressure measurements to be made at different depths in the well. During borehole construction of the 23 regional aquifer wells, at depths near 2,000 feet, the Laboratory has collected geologic samples (cuttings and core) for laboratory analysis; a complete suite of geophysical and video logs in the borehole; and water samples for contaminant screening.

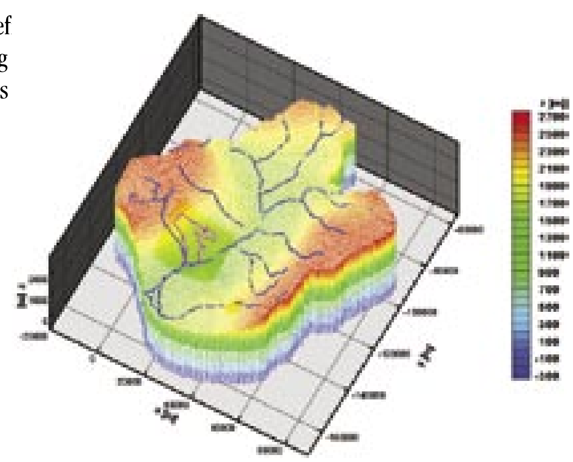
Each well is sampled 4 times during an 18-month period. The high-performance computing and modeling capabilities at Los Alamos are used to produce sophisticated models of the vadose zone and saturated zone. As a result, the Laboratory has derived a comprehensive understanding of the site's hydrogeologic setting.

## The Impact: Advanced Techniques to Solve Groundwater Resource Problems

After 6 years of implementing the Hydrogeologic Workplan, Los Alamos has been able to ref validate the conceptual model of the Pajarito Plateau hydrogeologic setting while increasing efficiency and cost effectiveness of the drilling process. In addition, data collection activities through the iterative DQO process have been enhanced. Another result has been the development of useful tools for performing risk assessments and protecting groundwater resources. The site-wide characterization has been completed ahead of the schedule.

Collaborating with regional government agencies and interested parties, the Laboratory is contributing its expertise and knowledge to solve problems on a regional basis in the Española Basin. Additionally, the experience gained by the Laboratory in conducting such a large-scale site investigation is directly transferable to other sites and locations, where it can be used to develop solutions for related ground-water resource management questions and problems.

Española Basin model 3-dimensional grid with Laboratory boundary highlighted, and elevations.



# Hydrogeologic Model of the Pajarito Plateau

## The Challenge: Collecting Data on the Pajarito Plateau Aquifer

Research on the hydrogeology of the Pajarito Plateau began as an outgrowth of the Rio Grande Project and the implementation of the Hydrogeologic Workplan for the Laboratory site. Driven by the need for a sound scientific basis to assess and manage groundwater resources, the Laboratory is conducting analyses of groundwater resources based on data collected from 23 deep monitoring/characterization wells in the regional aquifer across the Pajarito Plateau and from numerous existing wells located throughout the region.

## Los Alamos Innovation: Creating a Basin-Wide Model for Testing, Analysis, and Prediction

With its capabilities in geoscience, hydrology, modeling, risk management, and computational analysis, Los Alamos is well suited to create a 3-D model of the geologic framework and a sophisticated hydrologic model of the aquifer. The hydrologic model encompasses the entire Espanola Basin and includes

- Major stratigraphic units,
- Major water-cycle components,
- Topographic control on the watershed boundaries,
- Flow and transport components for both the vadose zone and the regional aquifer, and
- Accurate predictions of the combined impact of groundwater withdrawals from water users in the basin.

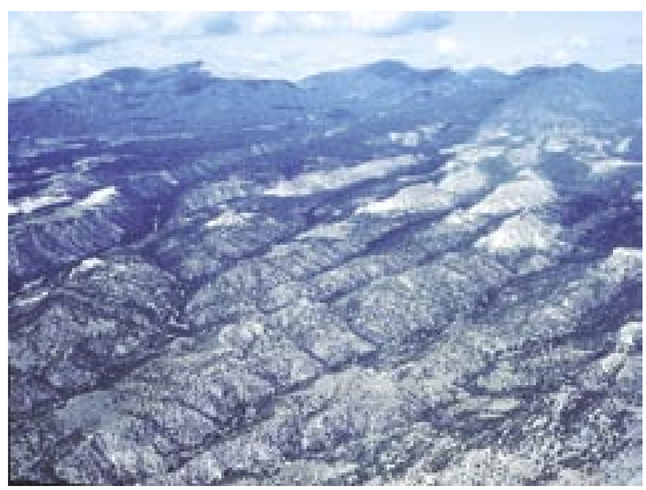
To maintain consistency in scientific approaches and provide technical recommendations to principal investigators and project managers, a Laboratory-wide Groundwater Integration Team (GIT) has been organized to serve as a technical peer review board and a collaborative configuration control board for technical information.

## The Impact: Insight on Groundwater Resources

Los Alamos's characterization's of the Pajarito Plateau is enhancing our understanding of the regional groundwater resources and the hydrogeologic setting in northern New Mexico. It is also helping Laboratory site environmental programs comply with regulations by estimating the fate of legacy contaminants in groundwater.

Los Alamos's models have also allowed for sighting sentry wells near water supply wells at risk of future contamination while providing insight into impacts of pumping municipal supply wells on the Pajarito Plateau and other existing wells in the basin. The modeling has also served surrounding communities and pueblos by illustrating and communicating water resource information and providing tools for making water resource management decisions.

The Laboratory is located on the Pajarito Plateau, which is made up of finger-like mesas separated by incised canyons.



# Understanding Uncertainty in Water Resource Prediction

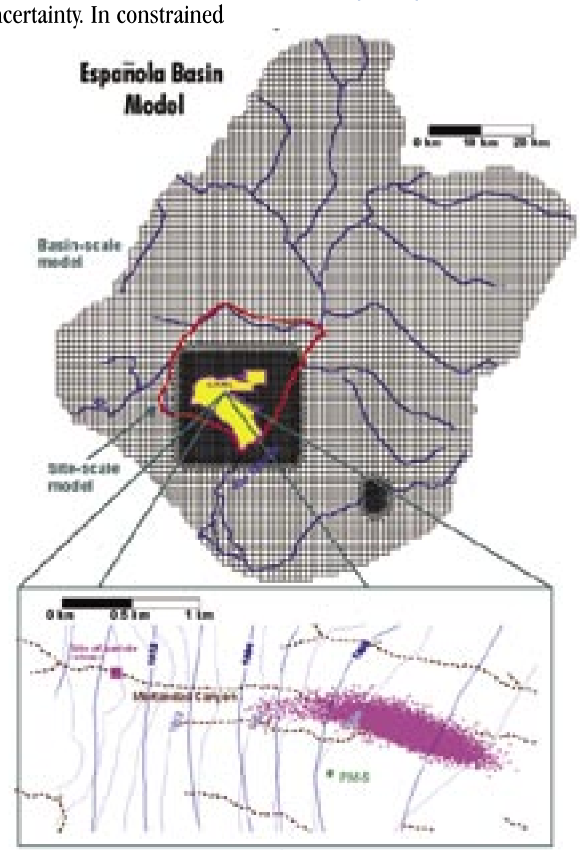
## The Challenge: Estimating Predictive Uncertainty in Water Resources Modeling

Models are widely used to understand and analyze behavior of physical systems and are particularly crucial to water resources research. Significant improvements in groundwater modeling capabilities have allowed for predictions based on more accurate simulations of complex processes. Relatively little attention, however, has been paid to a key aspect of model application: estimating predictive uncertainty. The uncertainty in predictions can be significant when models depend on uncertain knowledge about the modeled system and its governing processes. Los Alamos is developing new methodologies to provide not only water resource predictions, but also robust estimates of prediction uncertainty. Since models and their predictions are used widely in any decision-making process, careful analysis of model predictions and their uncertainty is of great importance to facilitate this process.

## Los Alamos Innovation: Developing Inverse Models to Quantify Uncertainty

Los Alamos has developed complex forward models, which predict system behavior given a set of model parameters, and complex inverse models, which estimate the model parameters (recharge rates, aquifer permeability) given a set of system measurements, i.e., calibration data (water levels in wells, streamflow measurements). To quantify the sensitivity and uncertainty in the calibrated inverse model is computationally intensive. Therefore, these models require robust information systems and complex coding, both of which are available and were developed at the Laboratory. Los Alamos uses two analytical approaches to the inverse model to quantify uncertainty. In constrained nonlinear optimization, plausible solutions are sought that maximize and minimize given model predictions, allowing prediction uncertainty to be quantified. In inverse-inverse analysis, which Los Alamos is developing, the set of calibration data required to produce a given model prediction with a specified degree of uncertainty

- Overcomes limitations associated with non-linearity of the forward model and non-normality and non linear correlation of the errors;
- Reveals the sensitivity of model parameters and predictions to the calibration data;
- Illuminates the impact of measurement error in calibration data on the inverse estimates and predictions; and
- Extends to quantify the sensitivity of inverse model estimates relevant to general system knowledge that can include the uncertainty caused by measurement or conceptual errors.




Plan view of model domains and grids. Inset shows a portion of the model where predictive uncertainty analysis of potential contaminant transport is performed.

## The Impact: Improving Diverse Modeling Efforts with Los Alamos Methodologies

The methodologies developed under this project estimate prediction uncertainties and identify key areas where improvements in our understanding of studied systems would decrease the uncertainty in the model predictions. The approaches developed under this project apply to a wide range of problems, including the Los Alamos Española Basin study, which deals with the aquifer in the Los Alamos region. Most of the national laboratories undertake projects that focus on developing models and making important predictions and conclusions using these models. As a result, the Los Alamos project is essential for the laboratories as they work toward the future of the nation.

# Plant Cover Effects on Water Resources

## The Challenge: Addressing Climate Change and Energy Issues

The United States Global Change Research Program (USGCRP) has identified the water and carbon cycles as national research priorities for the next 10 years. Within the water cycle, hydrological and ecological processes of dry land ecosystems are tightly interrelated. Many important relationships center on the effects that plant cover has on the water budget; for instance, changes in plant cover can trigger high rates of soil erosion. The Laboratory's involvement stems from addressing local environmental restoration needs, obtaining competitive grants within Los Alamos and DOE, and developing a terrestrial carbon sequestration program with the National Energy Technology Laboratory.

Los Alamos activities include

- Field experiments;
- Long-term monitoring of soil moisture, runoff, plant water stress, and ground cover;
- Simulation modeling;
- Analysis of historical aerial imagery; and
- Theory development.

The goal is to better quantify the interrelationships between vegetation pattern and dynamics with hydrological pattern and dynamics.

## Los Alamos Innovation: Plant Cover and Water Budget Relations

To achieve this goal, the Laboratory is applying its strengths in the area of plant cover and water budget relations. In conjunction with its capabilities in high-resolution hydrological modeling, the Laboratory offers

- The longest-term soil moisture data set for a semi-arid woodland;
- The best-documented example of a drought-induced ecotone shift;
- An experimental drought plot;
- The most intensely studied piñon-juniper woodland site; and
- Biophysical scaling relationships.

Mesita del Buey Woodland Research Site at Los Alamos National Laboratory, where a data set, spanning more than 15 years, has been compiled on soil water and associated plant relationships.

## The Impact: Real-World Applications

The Laboratory can use a variety of data in addressing diverse issues that include:

- Contaminant transport;
- Drought impacts management;
- Land use in semiarid environments;
- Global change impacts; and
- Terrestrial carbon management and sequestration.

# Improved Water Conservation with Waste Materials

## The Challenge: Using Plants to Reclaim Mine Sites and Manage Atmospheric Carbon

The United States Global Change Research Program has identified the carbon and water cycles as national research priorities, and the two cycles are strongly intertwined. Energy production and use, which is largely responsible for current imbalances in the carbon cycle, uses as much water as agriculture, and most of the costs of water treatment and distribution can be attributed to energy use. One part of achieving a sustainable water and energy future is the development of plants with optimal water efficiency. Because plants capture $CO_2$, a greenhouse gas, they play an important role in mitigating climate change. Water-efficient plants can serve double duty at the beginning and end of the energy cycle by revitalizing reclaimed mine sites and by capturing $CO_2$ produced by energy generation and use. A multidisciplinary team of Los Alamos researchers collaborated with site reclamation experts from the State of New Mexico Abandoned Mine Bureau and examined the potential of using coal mine site spoil and other waste materials to achieve improved vegetative growth and productivity.

## Los Alamos Innovation: Using Mine Waste Material as a Beneficial Soil Amendment

As Los Alamos researchers have pursued reclaiming western mine sites for vegetative growth, they have found that waste from western mine sites is high in nitrogen, but does not hold water well, making it a poor vegetation producer. Native western soil, on the other hand, contains clay and holds water well, but is low in nitrogen, making it a poor vegetation supporter. With their expertise in isotopic signatures and using a multidisciplinary approach, Los Alamos researchers have been able to distinguish carbon from coal from that derived from plants at mine sites. Los Alamos has also addressed the potential of using western mine site material to stabilize native alkaline soil to establish vegetative cover while combining native soil and mine site spoil to test its ability to support plant growth in water-limited regions.

Coal mine "gob" piles at Madrid, NM.

## The Impact: Plant Growth in Water-Limited Growth Systems

Results of this study reveal that native plants grown in combinations of coal mine spoil and native soil are outperforming those grown solely in native soil or solely in mine spoil. Further work in this area will lead to

- Reduced costs for mine site reclamation;
- More efficient water use when stabilizing reclaimed mine sites;
- Effective management of water in arid land where nitrogen is sparse;
- Beneficial use of waste materials; and
- Reduction in atmospheric carbon through plant capture and storage.

# Plants with Improved Water Use Efficiency

## The Challenge: Using Plants to Manage Atmospheric Carbon

Los Alamos has adopted a project to optimize the water efficiency of plants. This project is of special interest to two major U.S. industries: energy and agriculture. In addition to being the nation's largest users of water, the two industries are acutely interested in hardy, easily sustained plants for separate reasons. While agriculture has a keen financial interest in more water-efficient plants, the energy industry's particular interest is based on the role of plants in carbon sequestration. In the arid and semi-arid western United States, where precipitation is scarce, improving water efficiency is essential to using the natural ability of plants to capture $CO_2$ from greenhouse gas emissions.

## Los Alamos Innovation: Enhancing the Water Use Efficiency of Plants

Los Alamos has developed and patented a unique approach to enhancing the water use efficiency of plants. Because well-nourished plants require less water, the Laboratory has focused on developing plants that take up and use nutrients more efficiently.

Using the Laboratory's strengths in DNA sequence-based techniques in combination with isotope-assisted metabolic analysis, researchers developed the ability to manipulate plant growth by influencing the plant's own metabolic coordination of carbon and nitrogen. Researchers were also able to characterize the nutrient-use systems of a set of experimental plant systems and develop a prototype plant with improved nitrogen use and water use efficiencies.

## The Impact: More Efficient Crop Production and Control of Atmospheric Carbon

With results far beyond the original goals of the project and with the technical approaches applicable to both traditional and modern biotechnology, the generation of even more water efficient plants is possible. These plants could be expected to serve as a valuable part of carbon sequestration in the biosphere and to contribute to more water-efficient agricultural production.

Engineered plants with increased growth and water use efficiency.



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# Supercritical $CO_2$ Resist Removal (SCORR)

## The Challege: Reducing Water Use in Integrated Circuit Manufacturing

An integral step in integrated circuit manufacturing is photolithography. This step requires large amounts of hazardous solvents and vast amounts of ultra-pure deionized water. Along with 100,000 gallons of solvents, a single fabrication plant may use up to 4 million gallons of water per day to ensure that all traces of organic solvents and sulfates are removed from the wafer surface. Ironically, many of the largest plants in this country are located in states already plagued with chronic water and occasional energy shortages: New Mexico, California, Texas, and Arizona. Responding to a technical request from Hewlett Packard (now Agilent Technology), Los Alamos began developing the Supercritical $CO_2$ Resist Removal (SCORR) technology to address this problem.

Above: Scanning Electron Microscopy of via structure with residue from plasma etch processing.

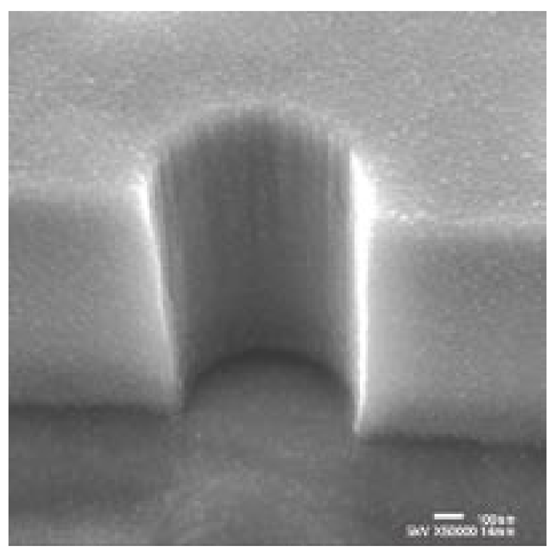
## Los Alamos Innovation: Using Supercritical Carbon Dioxide as a Replacement Solvent

To address this urgent problem facing the IC manufacturing industry, Los Alamos's SCORR technology met performance goals outlined in the International Technology Roadmap for Semiconductors, and rapidly evolved to commercial implementation. As a replacement solvent for integrated circuit manufacturing, SCORR can

- Greatly reduce or eliminate the use of water;
- Eliminate energy requirements for drying wafers and purifying water; and
- Reduce, by 95 to 99 percent, the use of hazardous chemicals (chlorofluorocarbon compounds, hydrogen peroxide, sulfuric acid, acetone, methyl-ethyl ketone and isopropyl alcohol.)

SCORR is a technically-enabling green process that is not only accepted but driven by leading semiconductor and IC manufacturers, as well as equipment and material suppliers.

Below: Scanning Electron Microscopy of plasma etch via structure followed by the SCORR process that has removed the residue material.



## The Impact: SCORR Will Enable Smaller Integrated Circuits and Other Nanotechnologies

To continue on their astounding growth curve, integrated circuits must become smaller, faster and cheaper. The International Technology Roadmap for Semiconductors details the technological barriers that need to be overcome in order to fabricate integrated circuits with diminishing feature sizes. Because of their high viscosity, the traditional liquid solvents presently being used will not be able to clean these small features. With SCORR, the smallest features present no barriers because supercritical fluids have zero surface tension and a gaslike viscosity, which allows them to remove particles smaller than 100 nanometers from integrated circuit features.

Los Alamos's developments in SCORR technology can enable industry to advance to increasingly finer architecture by removing a rate-limiting technical hurdle for the industry while cutting cost and nearly eliminating environmental liabilities. SCORR technology can also allow for the use of supercritical fluids to expand into many other fabrication processes and into other areas of nano-technology such as flat panel displays, Micro-Electro Mechanical (MEM) devices, and memory.

# Groundwater Remediation

## The Challenge: Cleaning Up Groundwater Pollution

Groundwater is a precious resource in New Mexico and elsewhere. After 50 years of serving the nation's defense needs, Los Alamos National Laboratory discovered that the alluvial (shallow) groundwater within nearby Mortandad Canyon had been contaminated with radionuclides, perchlorate, nitrate, and other inorganic chemicals. In response, Los Alamos developed the concept of multipermeable reactive barriers, which are designed to remove a variety of inorganic chemicals and radionuclides using natural materials. The materials were tested in the Laboratory prior to designing the Permeable Reactive Barrier (PRB) to be installed in Mortandad Canyon. The Mortandad Canyon field site was selected based on the nature and distribution of contaminants found in alluvial groundwater.

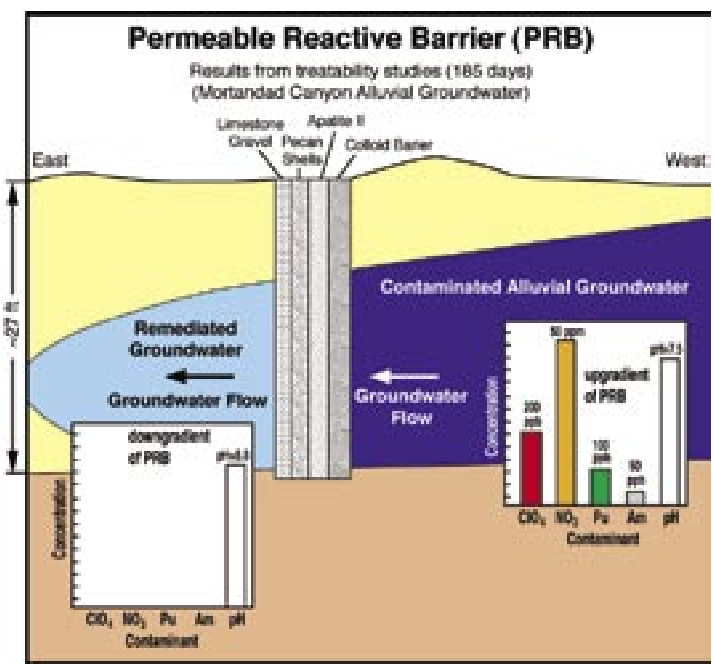
## Los Alamos Innovation: Combining Natural Materials to Remove Inorganic Contaminants

A multidisciplinary team was selected to work on the PRB project, integrating Los Alamos's capabilities in hydrology, geochemistry, geology, engineering, regulatory compliance, and computer modeling. The PRB is a passive system that eliminates the need to pump and treat contaminated alluvial groundwater, which is costly and ineffective for most inorganic chemicals and radionuclides. It also removes contaminants through adsorption, biodegradation and precipitation. It consists of natural materials (calcium hydroxylphosphate, cottonseed meal, pecan shells, and calcium carbonate) that achieve desired reactions with specific contaminants. As a result, radionuclides are removed by adsorbing onto calcium phosphate and coprecipitating with other metals and phosphate. Perchlorate is then biochemically reduced to chloride by cottonseed meal while nitrate is reduced to nitrogen gas under anaerobic conditions enhanced by cottonseed meal and carbonate, with a pH range between 7 and 8, neutralizing groundwater within the PRB.

## The Impact: Safe Groundwater in Norther New Mexico and Beyond

Since contaminated alluvial groundwater migrates through the subsurface and impacts deeper groundwater within Mortandad Canyon, removing perchlorate, nitrate, strontium-90, and other chemicals and radionuclides from alluvial groundwater within the canyon is most desirable. Installing the PRB will help to remediate alluvial groundwater, including the regional aquifer, and reduce the volume of contaminated groundwater migrating through the subsurface. PRB technology can be applied at other sites contaminated with metals, perchlorate, nitrate, radionuclides, and other inorganic contaminants.

Schematic cross section of the multiple permeable reactive barrier installed in Mortandad canyon.



# Scanning Raman LIDAR

## The Challenge: Accurate Measurement of Atmospheric Water Vapor

The U.S. Department of Defense requested that Los Alamos develop scanning LIDAR (Light Detection and Ranging) instruments to detect and monitor biological and chemical agents released into the atmosphere. An outgrowth of this program is the development of a scanning Raman water vapor LIDAR. Los Alamos built, tested, and fielded the scanning Raman LIDAR in an unprecedented 6 weeks.

The scanning LIDAR is an ideal tool for measuring eco-physiological parameters in the atmosphere, including the fate and transport of water vapor over agricultural and forested sites. It can also form the field support basis of integrated water and carbon cycle programs that will involve measurements and observations of water vapor and flux.

## Los Alamos Innovation: Using Laser Light for Specific Measurements

LIDAR operates in a manner similar to radar. A beam of energy is bounced off a distant object and the reflected energy is measured. However, LIDAR uses laser light instead of radio waves to scan distant objects. Because molecules interact with light in very specific ways, different wavelengths can be used to detect very specific chemical compounds, so water vapor can be isolated from other atmospheric gases.

The mobile scanning day/night Raman water vapor LIDAR has operated on both terrestrial and ocean surfaces. The most recent efforts have been concentrated on open water evapotranspiration at the Elephant Butte reservoir in southern New Mexico.

## The Impact: Understanding the Water and Carbon Cycles

The Laboratory's ongoing lidar research will help explain the spatial distribution of water vapor and flux in the atmosphere boundary layer (the region extending 1 kilometer into the atmosphere) while developing a water vapor and flux mapping system at an extremely high resolution in space. Because water vapor is the most abundant greenhouse gas and an important part of the global hydrological cycle, LIDAR will play a critical role in understanding and managing the interdependent water and carbon cycles.



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# Future Directions

## Water Management

The Earth's abundance of water belies its availability. While two-thirds of the planet is covered in water, only 2.5 percent is fresh, and only 1 percent is readily accessible. Pollution further reduces this number, and population increases mean more demand. With national security and global stability in mind, Los Alamos National Laboratory has identified the critical issues and the science and technology to address water problems in the United States and the World.

## Los Alamos National Laboratory Water Program Strategic Goals

**Water for Energy**
The energy industry is second only to agriculture in water use, and population growth strains water resources through both direct use and increased energy demand. Leading the way in identifying key challenges to energy and water supplies, Los Alamos engages industry and water regulators across the country, performing in-depth analyses to identify real-world problems and solutions, such as

- Decision support tools for water and energy policymakers,
- Technology to reduce water use,
- Access of untapped resources, and
- Water quality assurance.

Through industry and government partnership, solutions will move into the marketplace and planning community.

**Water Security**
Health and economic development depend heavily on the quantity and quality of water resources. Los Alamos is applying its expertise to homeland defense to address the new threats to a changing world. Los Alamos is improving its ability to predict, prevent, and respond to attacks on the nation's water supplies.

**Regional Water Cycle**
Los Alamos partners with universities, private industry, and government agencies to understand potential changes to water resources. Los Alamos is working with the atmospheric sciences community to develop models to simulate the global ocean and climate system. A detailed understanding of the climate response will allow regional simulations to assess local effects of climate variability and land use change. Integrated regional models, designed at Los Alamos, represent the atmosphere, landscape, and subsurface with accuracy, so locations and times for effective implementation of mitigating actions can be identified. Los Alamos is creating techniques to measure evaporation and water quality across basins, enhancing predictive capabilities and providing a better account of regional water. The results of this initiative will apply to future water use plans and will support water resource managers in their tasks.

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